Pyrrolidine

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.32e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.89e-01

Confidence level: 7.04e-01

Nearest Neighbors from the Training Set

Image not found
1-Propanethiol
Measured: 4.83e-11
Predicted: 3.35e-11

Image not found
1-Butanethiol
Measured: 5.10e-11
Predicted: 3.36e-11

Image not found
Bicyclo[2.2.1]heptane
Measured: 5.49e-12
Predicted: 1.23e-11

Image not found
Pentalene, octahydro-
Measured: 1.10e-11
Predicted: 1.77e-11

Image not found
2-Butanethiol
Measured: 4.00e-11
Predicted: 3.23e-11